

=> d his

(FILE 'HOME' ENTERED AT 03:20:47 ON 13 JUN 2007)

L1 FILE 'CAPLUS' ENTERED AT 03:20:56 ON 13 JUN 2007
1 S US2005-559857/APPS

FILE 'REGISTRY' ENTERED AT 03:21:13 ON 13 JUN 2007

L2 FILE 'CAPLUS' ENTERED AT 03:21:15 ON 13 JUN 2007
TRA L1 1- RN : 78 TERMS

L3 FILE 'REGISTRY' ENTERED AT 03:21:15 ON 13 JUN 2007
78 SEA L2

L4 FILE 'REGISTRY' ENTERED AT 03:59:21 ON 13 JUN 2007
STRUCTURE UPLOADED
L5 4 S L4

FILE 'STNGUIDE' ENTERED AT 04:00:06 ON 13 JUN 2007

L6 FILE 'REGISTRY' ENTERED AT 04:00:48 ON 13 JUN 2007
1668613 S NC4/ES
L7 0 S L4 SAM SUB=L6
L8 1899 S L4 SSS FULL SUB=L6
SAV TEM L8 BRD559857/A

L9 FILE 'CAPLUS' ENTERED AT 04:02:34 ON 13 JUN 2007
67 S L8

FILE 'STNGUIDE' ENTERED AT 04:03:04 ON 13 JUN 2007

FILE 'CAPLUS' ENTERED AT 04:03:24 ON 13 JUN 2007

=> d l4

L4 HAS NO ANSWERS

L4 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> d his

(FILE 'HOME' ENTERED AT 06:33:55 ON 13 JUN 2007)

L1 FILE 'CAPLUS' ENTERED AT 06:34:06 ON 13 JUN 2007
1 S US2005-559857/APPS

FILE 'STNGUIDE' ENTERED AT 06:35:08 ON 13 JUN 2007

FILE 'CAPLUS' ENTERED AT 06:38:27 ON 13 JUN 2007

FILE 'REGISTRY' ENTERED AT 06:38:40 ON 13 JUN 2007
ACT BRD559857/A

L2 STR
L3 (1668613)SEA FILE=REGISTRY ABB=ON PLU=ON NC4/ES
L4 1899 SEA FILE=REGISTRY SUB=L3 SSS FUL L2

FILE 'CAPLUS' ENTERED AT 06:38:51 ON 13 JUN 2007
L5 67 S L4
L6 1 S L1 AND L5

FILE 'REGISTRY' ENTERED AT 06:44:39 ON 13 JUN 2007
L7 STRUCTURE UPLOADED
L8 0 S L7 SAM SUB=L4

FILE 'STNGUIDE' ENTERED AT 06:45:25 ON 13 JUN 2007

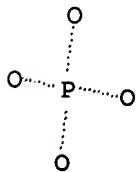
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L9 STRUCTURE UPLOADED
L10 1 S L9 SAM SUB=L4
L11 11 S L9 SSS FULL SUB=L4

FILE 'CAPLUS' ENTERED AT 06:47:39 ON 13 JUN 2007
L12 2 S L11

=> d 19

L9 HAS NO ANSWERS

L9 STR



Structure attributes must be viewed using STN Express query preparation.

=> d his

(FILE 'HOME' ENTERED AT 06:33:55 ON 13 JUN 2007)

L1 FILE 'CAPLUS' ENTERED AT 06:34:06 ON 13 JUN 2007
1 S US2005-559857/APPS

FILE 'STNGUIDE' ENTERED AT 06:35:08 ON 13 JUN 2007

FILE 'CAPLUS' ENTERED AT 06:38:27 ON 13 JUN 2007

FILE 'REGISTRY' ENTERED AT 06:38:40 ON 13 JUN 2007
ACT BRD559857/A

L2 STR
L3 (1668613)SEA FILE=REGISTRY ABB=ON PLU=ON NC4/ES
L4 1899 SEA FILE=REGISTRY SUB=L3 SSS FUL L2

FILE 'CAPLUS' ENTERED AT 06:38:51 ON 13 JUN 2007
L5 67 S L4
L6 1 S L1 AND L5

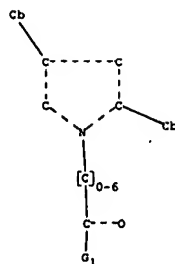
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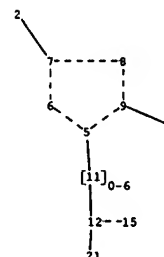
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L9 STRUCTURE UPLOADED
L10 1 S L9 SAM SUB=L4
L11 11 S L9 SSS FULL SUB=L4

FILE 'CAPLUS' ENTERED AT 06:47:39 ON 13 JUN 2007
L12 2 S L11
L13 0 S L5 AND KIM/IN
L14 17 S L5 AND KSP

=>



H 1 Ak 2



16 1 17 2

```

chain nodes :
  1  2 11 12 15 17 21
ring nodes :
  5  6  7  8  9
ring/chain nodes :
 16
chain bonds :
 1-9 2-7 5-11 11-12 12-15 12-21
ring bonds :
 5-6 5-9 6-7 7-8 8-9
exact/norm bonds :
 1-9 2-7 5-6 5-9 5-11 6-7 7-8 8-9 11-12 12-15 12-21
isolated ring systems :
  containing 5 :

```

G1:[*1],[*2]

Match level :

1:Atom 2:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 11:CLASS 12:CLASS
15:CLASS 16:CLASS 17:CLASS 21:CLASS

Generic attributes :

1:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic
2:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic
17:
Saturation : Saturated

Element Count :

Node 1: Limited
C,C6

Node 2: Limited
C,C6

=> d 112 tot bib abs hitstr

L12 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2006:188863 CAPLUS

DN 144:432640

TI Kinesin spindle protein (KSP) inhibitors. Part 3: Synthesis and evaluation of phenolic 2,4-diaryl-2,5-dihydropyrroles with reduced hERG binding and employment of a phosphate prodrug strategy for aqueous solubility

AU Garbaccio, Robert M.; Fraley, Mark E.; Tasber, Edward S.; Olson, Christy M.; Hoffman, William F.; Arrington, Kenneth L.; Torrent, Maricel; Buser, Carolyn A.; Walsh, Eileen S.; Hamilton, Kelly; Schaber, Michael D.; Fernandes, Christine; Lobell, Robert B.; Tao, Weikang; South, Vicki J.; Yan, Youwei; Kuo, Lawrence C.; Prueksaritanont, Thomayant; Slaughter, Donald E.; Shu, Cathy; Heimbrook, David C.; Kohl, Nancy E.; Huber, Hans E.; Hartman, George D.

CS Department of Medicinal Chemistry, Merck Research Laboratories, West Point, PA, 19486, USA

SO Bioorganic & Medicinal Chemistry Letters (2006), 16(7), 1780-1783

CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier B.V.

DT Journal

LA English

OS CASREACT 144:432640

AB 2,4-Diaryl-2,5-dihydropyrroles have been discovered to be novel, potent and water-soluble inhibitors of KSP, an emerging therapeutic target for the treatment of cancer. A potential concern for these basic KSP inhibitors was hERG binding that can be minimized by incorporation of a potency-enhancing C-2 phenol combined with neutral N-1 side chains. Aqueous solubility was restored to these, and other, non-basic inhibitors, through a phosphate prodrug strategy.

IT 812667-21-3P 812667-26-8P 884651-23-4P

884651-24-5P 884651-25-6P

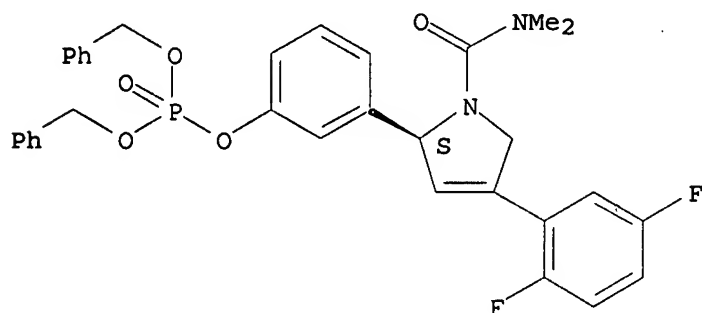
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 2,4-diaryl-2,5-dihydropyrroles as kinesin spindle protein (KSP) inhibitors with reduced hERG binding and phosphate prodrugs for aqueous solubility)

RN 812667-21-3 CAPLUS

CN Phosphoric acid, 3-[(2S)-4-(2,5-difluorophenyl)-1-[(dimethylamino)carbonyl]-2,5-dihydro-1H-pyrrol-2-yl]phenyl bis(phenylmethyl) ester (9CI) (CA INDEX NAME)

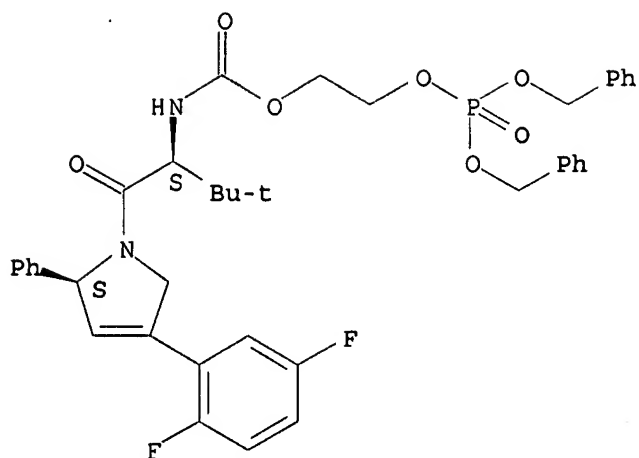
Absolute stereochemistry.



RN 812667-26-8 CAPLUS

CN Carbamic acid, [(1S)-1-[[[(2S)-4-(2,5-difluorophenyl)-2,5-dihydro-2-phenyl-1H-pyrrol-1-yl]carbonyl]-2,2-dimethylpropyl]-, 2-[[bis(phenylmethoxy)phosphinyl]oxy]ethyl ester (9CI) (CA INDEX NAME)

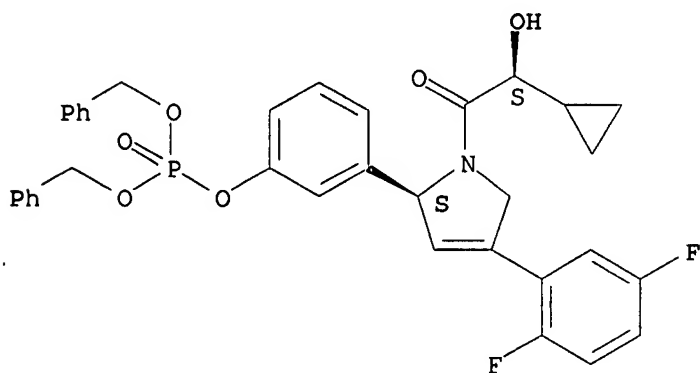
Absolute stereochemistry.



RN 884651-23-4 CAPLUS

CN Phosphoric acid, 3-[(2S)-1-[(2S)-cyclopropylhydroxyacetyl]-4-(2,5-difluorophenyl)-2,5-dihydro-1H-pyrrol-2-yl]phenyl bis(phenylmethyl) ester (9CI) (CA INDEX NAME)

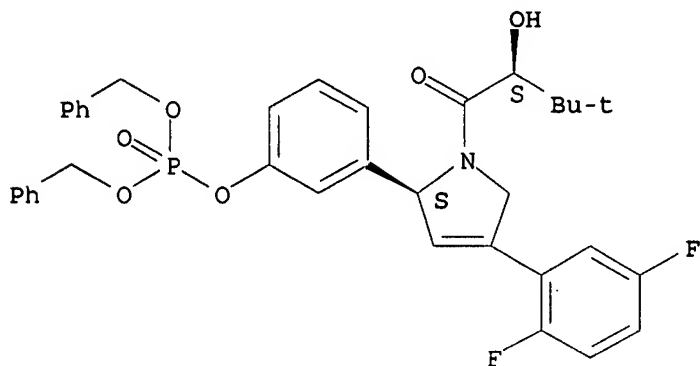
Absolute stereochemistry.



RN 884651-24-5 CAPLUS

CN Phosphoric acid, 3-[(2S)-4-(2,5-difluorophenyl)-2,5-dihydro-1-[(2S)-2-hydroxy-3,3-dimethyl-1-oxobutyl]-1H-pyrrol-2-yl]phenyl bis(phenylmethyl) ester (9CI) (CA INDEX NAME)

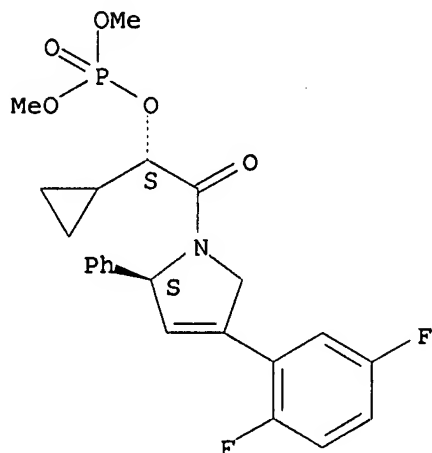
Absolute stereochemistry.



RN 884651-25-6 CAPLUS

CN Phosphoric acid, (1S)-1-cyclopropyl-2-[(2S)-4-(2,5-difluorophenyl)-2,5-dihydro-2-phenyl-1H-pyrrol-1-yl]-2-oxoethyl dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 812667-22-4P 812667-23-5P 812667-25-7P

812667-27-9P 812667-28-0P

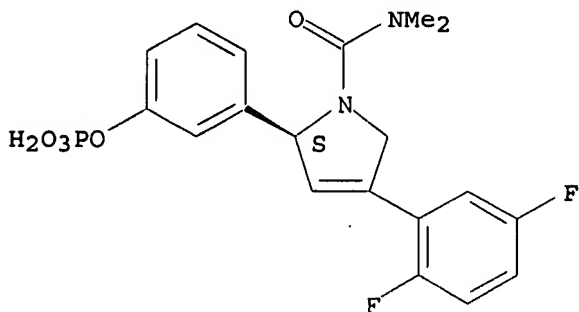
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of 2,4-diaryl-2,5-dihydropyrroles as kinesin spindle protein (KSP) inhibitors with reduced hERG binding and phosphate prodrugs for aqueous solubility)

RN 812667-22-4 CAPLUS

CN 1H-Pyrrole-1-carboxamide, 4-(2,5-difluorophenyl)-2,5-dihydro-N,N-dimethyl-2-[3-(phosphonooxy)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

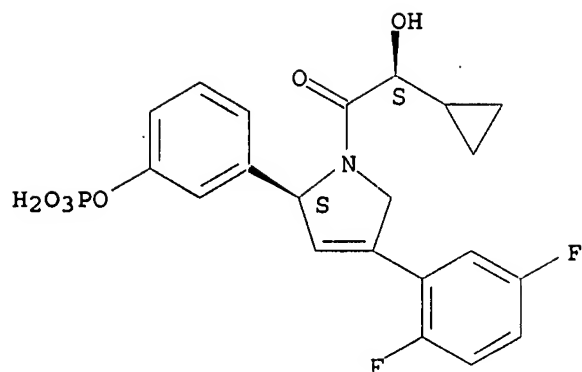
Absolute stereochemistry.



RN 812667-23-5 CAPLUS

CN 1H-Pyrrole, 1-[(2S)-cyclopropylhydroxyacetyl]-4-(2,5-difluorophenyl)-2,5-dihydro-2-[3-(phosphonooxy)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

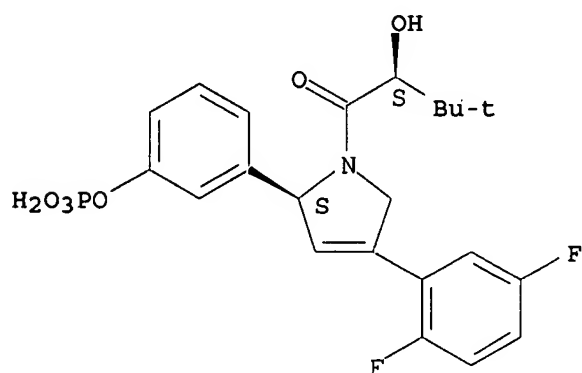
Absolute stereochemistry.



RN 812667-25-7 CAPLUS

CN 1H-Pyrrole, 4-(2,5-difluorophenyl)-2,5-dihydro-1-[(2S)-2-hydroxy-3,3-dimethyl-1-oxobutyl]-2-[3-(phosphonooxy)phenyl]-, (2S)-(9CI) (CA INDEX NAME)

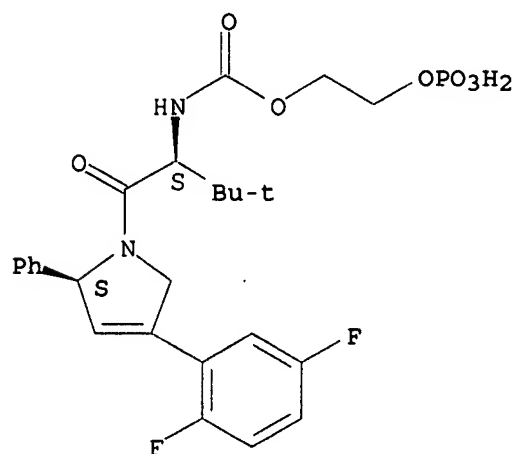
Absolute stereochemistry.



RN 812667-27-9 CAPLUS

CN Carbamic acid, [(1S)-1-[[[(2S)-4-(2,5-difluorophenyl)-2,5-dihydro-2-phenyl-1H-pyrrol-1-yl]carbonyl]-2,2-dimethylpropyl]-, 2-(phosphonooxy)ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

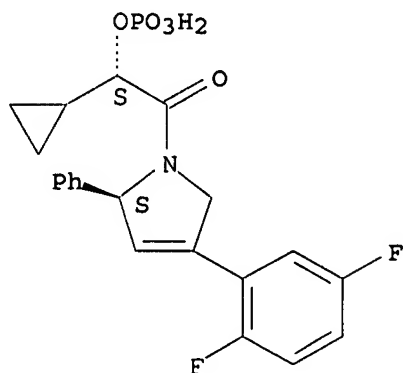


RN 812667-28-0 CAPLUS

CN 1H-Pyrrole, 1-[(2S)-cyclopropyl(phosphonooxy)acetyl]-4-(2,5-

difluorophenyl)-2,5-dihydro-2-phenyl-, (2S)- (9CI) (CA INDEX NAME)

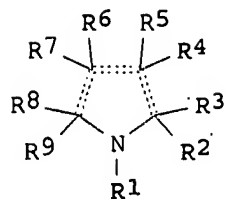
Absolute stereochemistry.



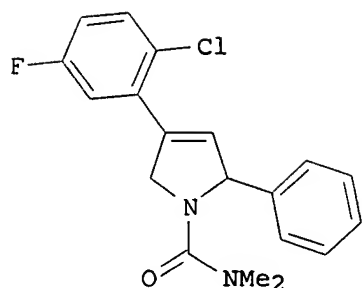
RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:1127483 CAPLUS
DN 142:74446
TI A preparation of pyrrole derivatives, useful as mitotic kinesin inhibitors
IN Fraley, Mark E.; Garbaccio, Robert M.; Hartman, George D.; Hoffman,
William F.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 112 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

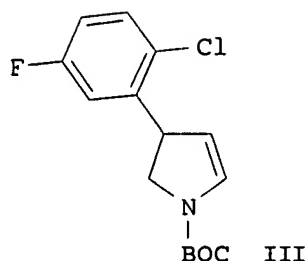
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004111193	A2	20041223	WO 2004-US18065	20040608
	WO 2004111193	A3	20050324		
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	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW:				
	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2004248160	A1	20041223	AU 2004-248160	20040608
	CA 2527582	A1	20041223	CA 2004-2527582	20040608
	EP 1636182	A2	20060322	EP 2004-754621	20040608
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	CN 1805928	A	20060719	CN 2004-80016354	20040608
	JP 2007505949	T	20070315	JP 2006-533588	20040608
	US 2006135594	A1	20060622	US 2005-559857	20051207
PRAI	US 2003-477995P	P	20030612		
	WO 2004-US18065	W	20040608		
OS	MARPAT 142:74446				
GI					



I



II



III

AB The invention relates to a preparation of pyrrole derivs. of formula I [wherein: R1 is (alkylene)0-1C(O)-alk(en/yn)yl, (alkylene)0-1C(S)-alk(en/yn)yl, or (alkylene)0-1-SO2-alkyl, etc.; R2 and R6 are independently selected from aryl, cycloalkyl, heterocyclyl, or aralkyl; R3, R4, R5, R7, R8, and R9 are independently selected from H, alk(en/yn)yl, aryl, or heterocyclyl, etc.], useful as mitotic kinesin inhibitors (no biol. data). The invention compds. are useful for the treatment of proliferative diseases such as cancer, hyperplasia, restenosis, and immune disorders. For instance, pyrrolocarboxamide derivative II was prepared via phenylation of N-BOC-pyrrol derivative III by $\text{PhN}_2 + \bullet\text{BF}_4^-$, N-deprotection, and N-carboxamidation by ClC(O)NMe_2 (scheme 1).

IT 812667-22-4P 812667-23-5P 812667-24-6P
812667-25-7P 812667-27-9P 812667-28-0P

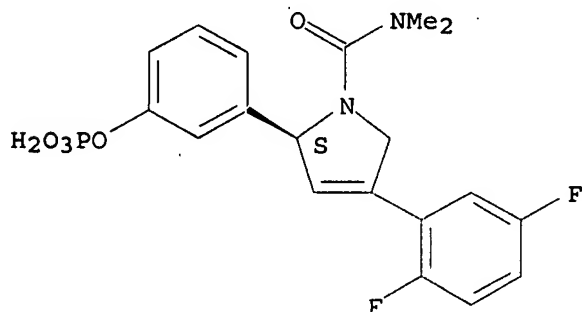
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

```
(preparation of pyrrole derivs. useful as mitotic kinesin inhibitors)
```

RN 812667-22-4 CAPLUS

CN 1H-Pyrrole-1-carboxamide, 4-(2,5-difluorophenyl)-2,5-dihydro-N,N-dimethyl-
2-[3-(phosphonooxy)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

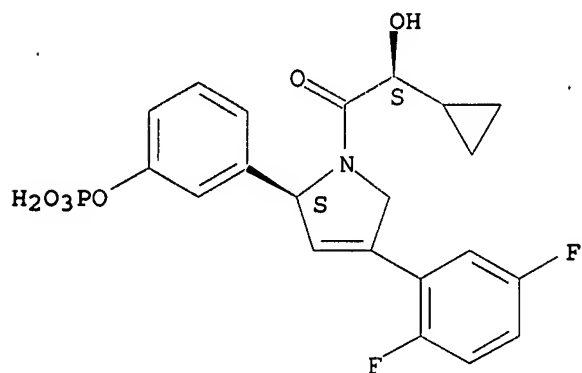


RN 812667-23-5 CAPLUS

CN 1H-Pyrrole, 1-[(2S)-cyclopropylhydroxyacetyl]-4-(2,5-difluorophenyl)-2,5-

dihydro-2-[3-(phosphonooxy)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

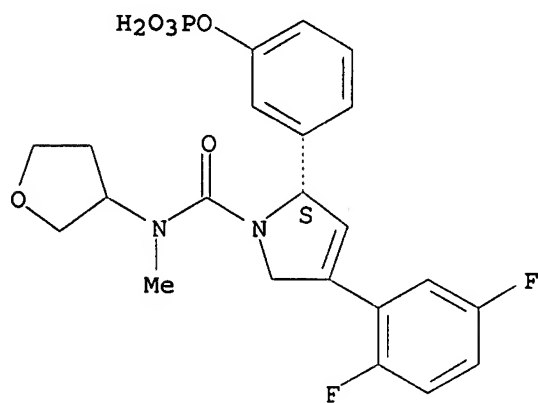
Absolute stereochemistry.



RN 812667-24-6 CAPLUS

CN 1H-Pyrrole-1-carboxamide, 4-(2,5-difluorophenyl)-2,5-dihydro-N-methyl-2-[3-(phosphonooxy)phenyl]-N-(tetrahydro-3-furanyl)-, (2S)- (9CI) (CA INDEX NAME)

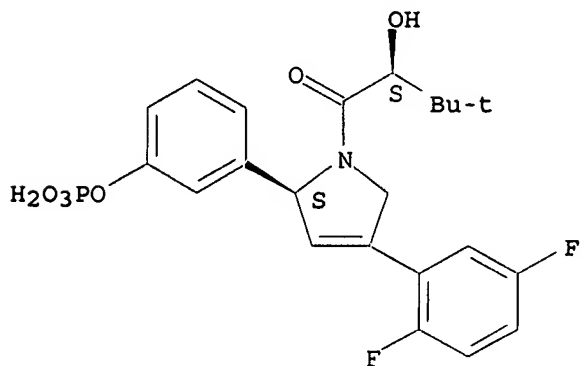
Absolute stereochemistry.



RN 812667-25-7 CAPLUS

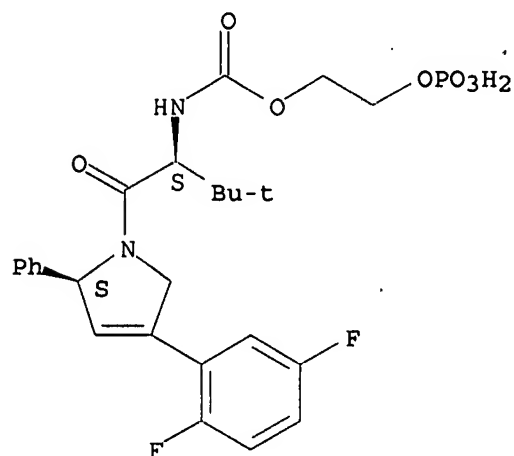
CN 1H-Pyrrole, 4-(2,5-difluorophenyl)-2,5-dihydro-1-[(2S)-2-hydroxy-3,3-dimethyl-1-oxobutyl]-2-[3-(phosphonooxy)phenyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



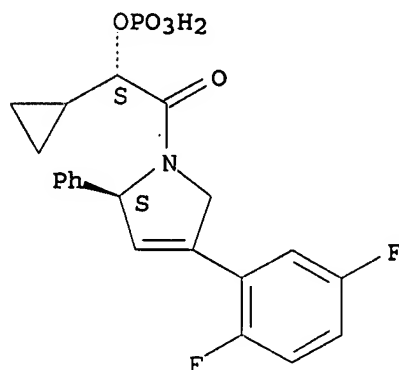
RN 812667-27-9 CAPLUS
 CN Carbamic acid, [(1S)-1-[[[(2S)-4-(2,5-difluorophenyl)-2,5-dihydro-2-phenyl-1H-pyrrol-1-yl]carbonyl]-2,2-dimethylpropyl]-, 2-(phosphonoxy)ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



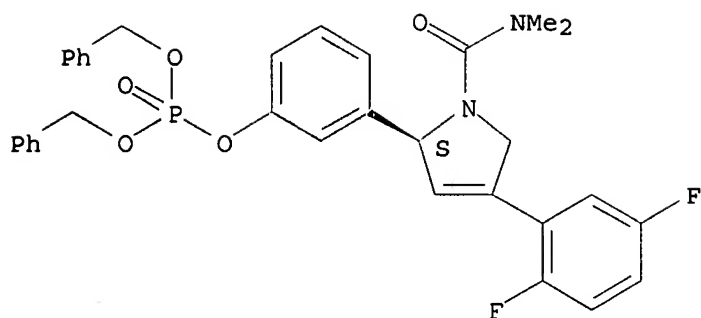
RN 812667-28-0 CAPLUS
 CN 1H-Pyrrole, 1-[(2S)-cyclopropyl(phosphonoxy)acetyl]-4-(2,5-difluorophenyl)-2,5-dihydro-2-phenyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 812667-21-3P 812667-26-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of pyrrole derivs. useful as mitotic kinesin inhibitors)
 RN 812667-21-3 CAPLUS
 CN Phosphoric acid, 3-[(2S)-4-(2,5-difluorophenyl)-1-[(dimethylamino)carbonyl]-2,5-dihydro-1H-pyrrol-2-yl]phenyl bis(phenylmethyl) ester (9CI) (CA INDEX NAME)

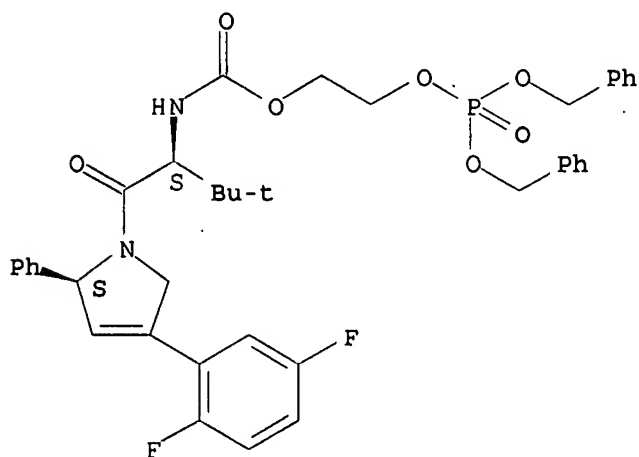
Absolute stereochemistry.



RN 812667-26-8 CAPLUS

CN Carbamic acid, [(1S)-1-[[[(2S)-4-(2,5-difluorophenyl)-2,5-dihydro-2-phenyl-1H-pyrrol-1-yl]carbonyl]-2,2-dimethylpropyl]-, 2-[[bis(phenylmethoxy)phosphinyl]oxy]ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> log hold

COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE ENTRY	TOTAL SESSION
11.01	69.22

SINCE FILE ENTRY	TOTAL SESSION
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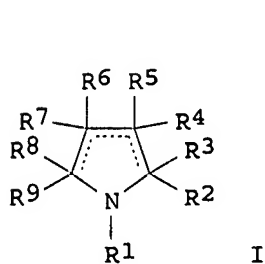
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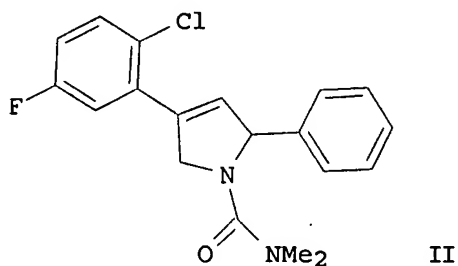
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L14 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:1006780 CAPLUS
DN 140:77020
TI Preparation of pyrrole derivatives as mitotic kinesin inhibitors
IN Arrington, Kenneth L.; Coleman, Paul J.; Cox, Christopher D.; Fraley, Mark E.; Garbaccio, Robert M.; Hartman, George D.; Hoffman, William F.; Tasber, Edward S.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 401 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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	AU 2003245453	A1	20031231	AU 2003-245453	20030612
	BR 2003011784	A	20050308	BR 2003-11784	20030612
	EP 1515724	A1	20050323	EP 2003-739093	20030612
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
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OS	MARPAT 140:77020				
GI					



I



II

AB The invention relates to dihydropyrrole compds. that are useful for treating cellular proliferative diseases and disorders associated with

KSP kinesin activity. The invention also relates to compns. which comprise these compds. and methods of using them to treat cancer in mammals. Compds. I [R1 is (C1-C6-alkylene)n-X-R, (n is 0 or 1; X is CO, SO2, NH, PO, etc.; R is alkyl, aryl, amino group, etc.), aryl, heterocyclyl, or alkyl; R2, R6 are aryl, aralkyl, cycloalkyl, or heterocyclyl; R3-R5, R7-R9 are H, alk(en)(yn)yl, aryl, aralkyl, heterocyclyl, etc.] (including amino acid derivs.) are claimed. For example, a detailed synthesis for the preparation of II is outlined, which includes reaction of 2 chloro-5-fluorobenzenediazonium tetrafluoroborate with Boc-protected 2,5-dihydro-1H-pyrrole-1-carboxylate.

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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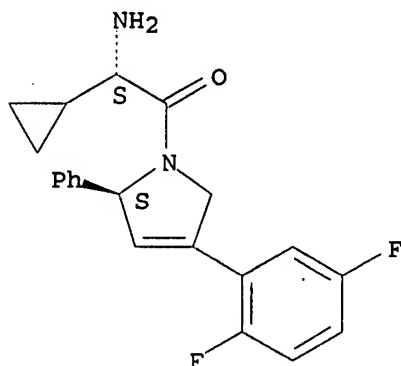
IT 639074-56-9 639074-88-7 639074-89-8
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812667-20-2 884902-56-1 884902-57-2
884902-58-3

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmacophore of KSP inhibitors)

RN 639074-56-9 CAPLUS

CN 1H-Pyrrole, 1-[(2S)-aminocyclopropylacetyl]-4-(2,5-difluorophenyl)-2,5-dihydro-2-phenyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 639074-88-7 CAPLUS

CN 1H-Pyrrole, 1-[(2S)-2-amino-3-methyl-1-oxobutyl]-4-(2,5-difluorophenyl)-2,5-dihydro-2-(3-hydroxyphenyl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

